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# On computational aspects of discrete Sobolev inner products on the unit circle

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## ABSTRACT

In this paper, we show how to compute in  $\mathcal{O}(n^2)$  steps the Fourier coefficients associated with the Gelfand Levitan approach for discrete Sobolev orthogonal polynomials on the unit circle when the support of the discrete component involving derivatives is located outside the closed unit disk. As a consequence, we deduce the outer relative asymptotics of these polynomials in terms of those associated with the original orthogonality measure. Moreover, we show how to recover the discrete part of our Sobolev inner product.

**Keywords:** Discrete Sobolev inner product, Gelfand–Levitan approach, Computational complexity, Cholesky decomposition, Outer relative asymptotics

## 1. Introduction

### 1.1. Orthogonal polynomials on the unit circle

Let us consider a non trivial probability measure  $d\sigma$  supported on the unit circle  $\mathbb{T} = \{z \in \mathbb{C}; |z| = 1\}$ . In the Hilbert space  $\mathcal{H} = L^2(\mathbb{T}, d\sigma)$  we define the usual inner product

$$(f, g) = \int_{\mathbb{T}} f(z) \overline{g(z)} d\sigma(z).$$

The application of the Gram–Schmidt process to  $1, z, z^2, \dots$ , yields a sequence of monic polynomials,  $\{\Phi_n(z)\}_{n \geq 0}$ , orthogonal with respect to the measure  $d\sigma(z)$ . In other words, there exists a unique sequence of monic polynomials, such that

$$\int_{\mathbb{T}} \Phi_n(z) \overline{\Phi_m(z)} d\sigma(z) = \kappa_n^2 \delta_{n,m}, \quad \kappa_n > 0, \quad n, m \geq 0,$$

where  $\delta_{n,m}$  is the Kronecker delta, and

$$\kappa_n^2 = \|\Phi_n\|^2 = \int_{\mathbb{T}} |\Phi_n(z)|^2 d\sigma(z).$$

Let us denote by  $\phi_n(z) = \kappa_n \Phi_n(z)$  the orthonormal polynomial of degree  $n$  with respect to  $d\sigma(z)$ . According to Fejér's theorem [15, 16], if  $\alpha$  is a zero of  $\phi_n(z)$  then  $|\alpha| < 1$ .

It is well known that the sequence  $\{\Phi_n(z)\}_{n \geq 0}$  satisfies the following forward and backward recurrence relations

$$[16, 15] \quad \Phi_{n+1}(z) = z\Phi_n(z) + \Phi_{n+1}(0)\Phi_n^*(z), \quad n \geq 0, \quad (1.1)$$

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$$\Phi_{n+1}(z) = \left(1 - |\Phi_{n+1}(0)|^2\right) z \Phi_n(z) + \Phi_{n+1}(0) \Phi_{n+1}^*(z), \quad n \geq 0, \quad (1.2)$$

where  $\Phi_n^*(z) = \overline{z^n \Phi_n(z)}$  is the so called reversed polynomial, and the complex numbers  $\{\Phi_n(0)\}_{n \geq 1}$ , with

$$|\Phi_n(0)| < 1, \quad n \geq 1, \quad (1.3)$$

are known in the literature (see [15]) as Verblunsky, Schur, or reflection coefficients. The monic orthogonal polynomials are therefore completely determined by the sequence  $\{\Phi_n(0)\}_{n \geq 1}$ . In this situation, we have an analogous of Favard's theorem [15,16], formulated as follows. Any sequence  $\{a_n\}_{n \geq 1}$  of complex numbers satisfying  $|a_n| < 1$  for every  $n \geq 1$  arises as the sequence of Verblunsky coefficients of a unique non trivial probability measure supported on the unit circle.

In the case of orthogonal polynomials on the unit circle we have a simple expression for the polynomial kernel [15,16], similar to the Christoffel Darboux formula on the real line [5]. The  $n$ th polynomial kernel  $K_n(z, y)$  associated with  $\Phi_n(z)$  is given by

$$K_n(z, y) = \sum_{j=0}^n \frac{\overline{\Phi_j(y)} \Phi_j(z)}{\|\Phi_j\|^2} = \frac{\overline{\Phi_{n+1}(y)} \Phi_{n+1}^*(z) - \overline{\Phi_{n+1}(y)} \Phi_{n+1}(z)}{\|\Phi_{n+1}\|^2 (1 - y\bar{z})}, \quad (1.4)$$

and it satisfies the reproducing property,

$$\int_{\mathbb{T}} K_n(z, y) \overline{f(z)} d\sigma(z) = \overline{f(y)}, \quad (1.5)$$

for every polynomial  $f$  of degree at most  $n$ .

The orthogonality measure can be decomposed as the sum of a purely absolutely continuous measure with respect to the Lebesgue measure and a singular part. Thus, if we denote by  $\sigma'(\theta)$ , the Radon Nikodym derivative of the measure  $\sigma(\theta)$  supported in  $[\pi, \pi]$  with respect to the Lebesgue measure, then

$$d\sigma(\theta) = \sigma'(\theta) \frac{d\theta}{2\pi} + d\sigma_s(\theta), \quad (1.6)$$

where  $\sigma_s(\theta)$  is the singular part of  $\sigma(\theta)$ .

In the literature, two of the most relevant classes of measures are the Szego" and Nevai class. We say that  $d\sigma(\theta)$  belongs to the Szego" class if

$$\int_{\pi}^{\pi} \log \sigma'(\theta) \frac{d\theta}{2\pi} > -\infty,$$

i.e.,  $\log \sigma'(z) \in L^1[\pi, \pi]$ .

On the other hand, we say that  $d\sigma(\theta)$  belongs to the Nevai class if

$$\lim_{n \rightarrow \infty} \Phi_n(0) = \lim_{n \rightarrow \infty} \frac{\Phi_n(0)}{\kappa_n} = 0.$$

The relation between the above two classes can be viewed using the results contained in [13].

## 1.2. Discrete Sobolev orthogonal polynomials

In the last years, some attention has been paid to the study of asymptotic properties of orthogonal polynomials with respect to non standard inner products. More precisely, several authors have focused their interest on sequences of polynomials orthogonal with respect to Sobolev inner products (see [12] for an updated overview with more than 350 references). Their algebraic and analytic properties of orthogonal polynomials associated with a particular case of Sobolev inner product, the so called discrete case, have been intensively studied. The asymptotic behavior of such sequences of orthogonal polynomials, the localization, interlacing properties, asymptotic behavior and monotonicity of their zeros, Fourier expansions as well as their relevance in the analysis of spectral methods for boundary value problems in the theory of partial differential equations provide a very large field to explore.

The aim of this contribution is to study computational aspects of polynomials  $\{\psi_n(z)\}_{n \geq 0}$  which are orthonormal with respect to the discrete Sobolev inner product

$$\langle f, g \rangle = \int_{\mathbb{T}} f(z) \overline{g(z)} d\sigma(z) + \sum_{k=0}^N M_k f^{(l_k)}(z_k) \overline{g^{(l_k)}(z_k)}, \quad M_k > 0, z_k \in \mathbb{C}, \quad (1.7)$$

where  $l_k, k = 0, 1, \dots, N$ , are non negative integer numbers. To the best of our knowledge, the computational aspects of Sobolev inner products have not been studied previously up to for the real line case in an unpublished manuscript due to Van Assche [17], and the contributions [7,18]. We follow the same schedule and uses the same ideas given in the manuscript [17]. The paper and the manuscript contain similar results with only few changes which are related with the support of the measure and the asymptotic properties of the sequence of orthogonal polynomials.

We recall that more general inner products where cross derivatives appear in the discrete part of (1.7) have been also studied. Moreover, the sequences of orthonormal polynomials in the non diagonal case have the same outer asymptotic behavior as the corresponding to the diagonal case, see [3]. In such a situation, a more precise information can be done. The asymptotic behavior does not depend on the masses  $M_k$ ,  $k = 0, 1, \dots, N$ , see, among others, [2,10,11].

The structure of the manuscript is as follows. In Section 2, we obtain in  $\mathcal{O}(n^3)$  steps through a Cholesky decomposition of the corresponding Gram matrix, the Fourier coefficients associated with the Gelfand Levitan approach for discrete Sobolev orthogonal polynomials on the unit circle. In Section 3, we reduce the computational complexity to  $\mathcal{O}(n^2)$  steps. In Section 4, we find a way to recover the discrete part of our Sobolev inner product using the asymptotic behavior of the corresponding sequence of orthogonal polynomials. Finally, we also propose some related open problems.

## 2. The Gelfand–Levitan approach

Basically, the Gelfand–Levitan approach is based on the fact that the polynomial  $\psi_n(z)$  of degree  $n$ , orthonormal with respect to the Sobolev inner product (1.7) can be considered as a perturbation of  $\phi_n(z)$ . Hence, useful information can be obtained by expanding  $\psi_n(z)$  in an orthonormal series

$$\psi_n(z) = \sum_{k=0}^n \lambda_{n,k} \phi_k(z), \quad n \geq 0. \quad (2.8)$$

This approach can be traced back to Bernstein for orthogonal polynomials on  $[1, 1]$  and probably Bernstein's method inspired to Gelfand and Levitan to work out a similar procedure for the analysis of differential equations from its spectral function [8].

It is clear that the knowledge of the Fourier coefficients  $\lambda_{j,k}$ ,  $0 \leq k \leq j$ ,  $0 \leq j \leq n$ , is the key to understand the behavior of the sequence of discrete Sobolev orthonormal polynomials  $\{\psi_n\}_{n \geq 0}$ .

Let us introduce the lower triangular matrix

$$\mathbb{L}_n = \begin{bmatrix} \lambda_{0,0} & 0 & \cdots & 0 \\ \lambda_{1,0} & \lambda_{1,1} & 0 & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{n,0} & \lambda_{n,1} & \cdots & \lambda_{n,n} \end{bmatrix}, \quad (2.9)$$

of order  $(n+1) \times (n+1)$ . Therefore, (2.8) can be represented in a matrix form as

$$\psi_n(z) = \mathbb{L}_n \phi_n(z), \quad (2.10)$$

where

$$\begin{bmatrix} \psi_0(z) \\ \psi_1(z) \\ \vdots \\ \psi_n(z) \end{bmatrix} = \begin{bmatrix} \lambda_{0,0} & 0 & \cdots & 0 \\ \lambda_{1,0} & \lambda_{1,1} & 0 & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{n,0} & \lambda_{n,1} & \cdots & \lambda_{n,n} \end{bmatrix} \begin{bmatrix} \phi_0(z) \\ \phi_1(z) \\ \vdots \\ \phi_n(z) \end{bmatrix} \quad \text{and } {}^T \text{ denote the transpose. Let } \mathbb{G}_n = \begin{bmatrix} \langle \phi_0(z), \phi_0(z) \rangle & \langle \phi_0(z), \phi_1(z) \rangle & \cdots & \langle \phi_0(z), \phi_n(z) \rangle \\ \langle \phi_1(z), \phi_0(z) \rangle & \langle \phi_1(z), \phi_1(z) \rangle & \cdots & \langle \phi_1(z), \phi_n(z) \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \phi_n(z), \phi_0(z) \rangle & \langle \phi_n(z), \phi_1(z) \rangle & \cdots & \langle \phi_n(z), \phi_n(z) \rangle \end{bmatrix}$$

be the Gram matrix associated with the sequence of orthonormal polynomials  $\{\phi_n(z)\}_{n \geq 0}$ . From (2.10), we obtain

$$\langle \psi_n(z), \phi_n(z) \rangle = \mathbb{L}_n \mathbb{G}_n, \quad (2.11)$$

where

$$\langle \psi_n(z), \phi_n(z) \rangle = \begin{bmatrix} \langle \psi_0(z), \phi_0(z) \rangle & \langle \psi_0(z), \phi_1(z) \rangle & \cdots & \langle \psi_0(z), \phi_n(z) \rangle \\ \langle \psi_1(z), \phi_0(z) \rangle & \langle \psi_1(z), \phi_1(z) \rangle & \cdots & \langle \psi_1(z), \phi_n(z) \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \psi_n(z), \phi_0(z) \rangle & \langle \psi_n(z), \phi_1(z) \rangle & \cdots & \langle \psi_n(z), \phi_n(z) \rangle \end{bmatrix} \text{ Since } \mathbb{L}_n \text{ is non singular, from (2.10) we also find}$$

$$\phi_n(z) = \mathbb{L}_n^{-1} \psi_n(z),$$

so that

$$\langle \psi_n(z), \phi_n(z) \rangle = \langle \psi_n(z), \mathbb{L}_n^{-1} \psi_n(z) \rangle = \langle \psi_n(z), \psi_n(z) \rangle \mathbb{L}_n^{-1} \left( \begin{matrix} 1 \\ 0 \\ \vdots \\ 0 \end{matrix} \right) (\mathbb{L}_n^H)^H,$$

where  $^H$  denote the transpose conjugate. Thus, solving (2.11) for  $\mathbb{G}_n$  we get the following result.

**Lemma 2.1.** *Let  $\mathbb{G}_n$  be the Gram matrix of the inner product (1.7) associated with the sequence of orthonormal polynomials  $\{\phi_n(z)\}_{n \geq 0}$ . Then,*

$$\mathbb{G}_n = \mathbb{L}_n^{-1} (\mathbb{L}_n^{-1})^H,$$

where  $\mathbb{L}_n$  is the lower triangular matrix defined in (2.9).

Taking into account that  $\mathbb{L}_n^{-1}$  is a lower triangular matrix and  $(\mathbb{L}_n^{-1})^H$  is an upper triangular matrix which is equal to the transpose of  $\mathbb{L}_n^{-1}$ , Lemma 2.1 yields the Cholesky decomposition of the Gram matrix  $\mathbb{G}_n$ . In other words, we get a straightforward numerical method based on numerical linear algebra for obtaining the Fourier coefficients  $\lambda_{j,k}$ ,  $0 \leq k \leq j, j \leq n$ , in  $\mathcal{O}(n^3)$  steps. A natural question is: can we reduce this complexity? An affirmative answer is given in the next section.

### 3. Reducing the computational complexity

The entries in the Gram matrix  $\mathbb{G}_n$  are explicitly given by

$$\langle \phi_i(z), \phi_j(z) \rangle = \int_{\mathbb{T}} \phi_i(z) \overline{\phi_j(z)} d\sigma(z) + \sum_{k=0}^N M_k \phi_i^{(l_k)}(z_k) \overline{\phi_j^{(l_k)}(z_k)} = \delta_{ij} + \sum_{k=0}^N M_k \phi_i^{(l_k)}(z_k) \overline{\phi_j^{(l_k)}(z_k)}, \quad 0 \leq i, j \leq n,$$

where the evaluation of orthonormal polynomials  $\{\phi_n(z)\}_{n \geq 0}$  in the support of the discrete part of the inner product appears. Thus we can write

$$\mathbb{G}_n = \mathbb{I}_n + \mathbb{S}_n,$$

where  $\mathbb{I}_n$  is the identity matrix, and the entries of  $\mathbb{S}_n$  are

$$(\mathbb{S}_n)_{ij} = \sum_{k=0}^N M_k \phi_i^{(l_k)}(z_k) \overline{\phi_j^{(l_k)}(z_k)}, \quad 0 \leq i, j \leq n. \quad (3.12)$$

From Lemma 2.1,

$$(\mathbb{L}_n^{-1})^H = \mathbb{L}_n + \mathbb{L}_n \mathbb{S}_n.$$

Therefore, for  $m < n$  and taking into account the last row of the matrices involved in the above identity, we get

$$0 = \lambda_{n,m} + \sum_{k=0}^n M_k (\mathbb{S}_n)_{k,m}, \quad 0 \leq m \leq n-1. \quad (3.13)$$

When  $n = m$ ,

$$\frac{1}{\lambda_{n,n}} = \lambda_{n,n} + \sum_{k=0}^n M_k (\mathbb{S}_n)_{k,n}. \quad (3.14)$$

From (3.12), we see that  $(\mathbb{S}_n)_{ij}$ ,  $0 \leq i, j \leq n$ , has a special form in which the variables  $i$  and  $j$  are separated in each term of the sum. This structure suggests that a similar separation of indices should also hold for the Fourier coefficients.

**Theorem 3.1.** *Let  $\mathbb{K}_{n-1}$  be the kernel matrix with entries*

$$(\mathbb{K}_{n-1})_{ij} = \sum_{k=0}^{n-1} \phi_k^{(l_i)}(z_i) \overline{\phi_k^{(l_j)}(z_j)}, \quad 0 \leq i, j \leq n-1, \quad (3.15)$$

and, let  $\mathbf{a}_n = [a_{n,0}, a_{n,1}, \dots, a_{n,N}]^T$  be the solution of the linear system of equations

$$(\mathbb{I}_N + \mathbb{K}_{n-1} \mathbb{D}_N) \mathbf{a}_n = \mathbf{b}_n, \quad (3.16)$$

where  $\mathbb{D}_N = \text{diag } M_0, M_1, \dots, M_N$  and  $\mathbf{b}_n = [\phi_n^{(l_0)}(z_0), \phi_n^{(l_1)}(z_1), \dots, \phi_n^{(l_N)}(z_N)]^T$ . Then, for all  $n \geq 0$ , we have

$$\frac{\lambda_{n,k}}{\lambda_{n,n}} = \sum_{i=0}^N M_i \phi_k^{(l_i)}(z_i), \quad 0 \leq k \leq n-1 \quad (3.17)$$

and

$$\frac{1}{\lambda_{n,n}^2} = 1 + \sum_{i=0}^N M_i \phi_n^{(l_i)}(z_i). \quad (3.18)$$

**Proof.** In order to prove the above statements we need to show that (3.17) and (3.18) satisfy (3.13) and (3.14). If we use the proposed solution (3.17), then we find

$$\frac{\lambda_{n,m}}{\lambda_{n,n}} + \sum_{k=0}^n \frac{\lambda_{n,k}}{\lambda_{n,n}} (\mathbb{S}_n)_{k,m} = \sum_{i=0}^N \overline{a_{n,i} M_i \phi_m^{(l_i)}(z_i)} + \sum_{k=0}^n \frac{1}{\lambda_{n,n}} (\mathbb{S}_n)_{k,m} \sum_{i=0}^N \overline{a_{n,i} M_i \phi_k^{(l_i)}(z_i)} + (\mathbb{S}_n)_{n,m}.$$

By using the explicit expression for  $(\mathbb{S}_n)_{k,m}$ ,  $0 \leq k \leq n$ , this becomes

$$\frac{\lambda_{n,m}}{\lambda_{n,n}} + \sum_{k=0}^n \frac{\lambda_{n,k}}{\lambda_{n,n}} (\mathbb{S}_n)_{k,m} = \sum_{i=0}^N \overline{a_{n,i} M_i \phi_m^{(l_i)}(z_i)} + \sum_{k=0}^n \frac{1}{\lambda_{n,n}} \sum_{j=0}^N \overline{a_{n,j} M_j \phi_k^{(l_j)}(z_j)} \left( \sum_{i=0}^N \overline{M_i \phi_k^{(l_i)}(z_i) \phi_n^{(l_i)}(z_i)} \right) + \sum_{i=0}^N \overline{M_i \phi_n^{(l_i)}(z_i) \phi_m^{(l_i)}(z_i)}.$$

Combining all the terms where the values  $\overline{\phi_n^{(l_i)}(z_i)}$ ,  $i = 0, 1, \dots, N$ , appear, the above expression yields

$$\frac{\lambda_{n,m}}{\lambda_{n,n}} + \sum_{k=0}^n \frac{\lambda_{n,k}}{\lambda_{n,n}} (\mathbb{S}_n)_{k,m} = \sum_{i=0}^N \overline{M_i \phi_m^{(l_i)}(z_i)} a_{n,i} + \sum_{k=0}^n \sum_{j=0}^N \overline{a_{n,j} M_j \phi_k^{(l_j)}(z_j) \phi_k^{(l_j)}(z_j)} + \phi_n^{(l_i)}(z_i).$$

Notice that the expression inside brackets is the  $i$ th equation in the linear system of Eq. (3.16). Hence, this expression vanishes and (3.13) is satisfied.

It remains now to determine the value of  $\lambda_{n,n}$  which can be done using (3.14), as follows

$$\frac{1}{\lambda_m^2} = 1 + \sum_{k=0}^n \frac{\lambda_{n,k}}{\lambda_{n,n}} (\mathbb{S}_n)_{k,n} + (\mathbb{S}_n)_{n,n}.$$

By using the explicit expression of  $(\mathbb{S}_n)_{k,n}$ ,  $0 \leq k \leq n$ , and the solution (3.17) the previous identity becomes

$$\frac{1}{\lambda_m^2} = 1 + \sum_{k=0}^n \sum_{i=0}^N \overline{a_{n,i} M_i M_j \phi_k^{(l_j)}(z_j) \phi_k^{(l_i)}(z_i) \phi_n^{(l_i)}(z_i)} + \sum_{j=0}^N \overline{M_j |\phi_n^{(l_j)}(z_j)|^2}.$$

From the linear system of Eq. (3.16), we find

$$\sum_{i=0}^N \overline{M_i a_{n,i} (\mathbb{K}_{n-1})_{j,i}} = a_{n,j} \phi_n^{(l_j)}(z_j).$$

Thus,

$$\frac{1}{\lambda_m^2} = 1 + \sum_{j=0}^N \overline{M_j} \left( a_{n,j} + \phi_n^{(l_j)}(z_j) \overline{\phi_n^{(l_j)}(z_j)} \right) + \sum_{j=0}^N \overline{M_j} |\phi_n^{(l_j)}(z_j)|^2 = 1 + \sum_{j=0}^N \overline{M_j} a_{n,j} \phi_n^{(l_j)}(z_j),$$

which corresponds to (3.18).  $\square$

Here we recall a well known result [6] concerning the relation between the algebraic expressions of both families of orthogonal polynomials  $\phi_n(z)$  and  $\psi_n(z)$ . Indeed, this is the standard way to obtain the linear system of Eq. (3.16).

Notice that we have reduced the computation of the Fourier coefficients  $\lambda_{j,k}$ ,  $0 \leq k \leq j, j \leq n$ , to solve the linear system of Eq. (3.16). The next step is to evaluate the polynomials  $\phi_n(z)$  and some of their derivatives at the  $N+1$  points  $z_k$ ,  $k = 0, 1, \dots, N$ . This can be done in  $\mathcal{O}(n(N+1))$  steps by using the recurrence relation (1.1). The kernel matrix  $\mathbb{K}_{n-1}$  can be obtained from the Christoffel-Darboux formula (1.4) in  $\mathcal{O}(N+1)^2$  steps. Thus,  $\lambda_{n,k}$ ,  $k = 0, 1, \dots, n$ , can be computed in  $\mathcal{O}(n)$  steps whenever  $N$  is finite. As a consequence, we reduce the required computing time to calculate the complete array of Fourier coefficients.

**Corollary 3.1.** To compute the Fourier coefficients  $\lambda_{j,k}$ ,  $0 \leq k \leq j, j \leq n$ , we require  $\mathcal{O}(n^2)$  operations.

The kernel matrix  $\mathbb{K}_{n-1}$  given in (3.15) satisfies an interesting extremal property, which was first observed by Grenander and Rosenblatt [9] motivated by their applications in the theory of stationary stochastic processes.

Let denote by  $\mathbb{P}_{n-1}$  the linear space of polynomials with complex coefficients and degree at most  $n-1$  and let

$$\|X_{n-1}\|^2 = \int_{\mathbb{T}} |X_{n-1}(z)|^2 d\sigma(z),$$

be the squared norm of the polynomial  $X_{n-1}(z) \in \mathbb{P}_{n-1}$  in the linear space  $\mathcal{H} = L^2(\mathbb{T}, d\sigma)$ . If one imposes the constraints

$$X_{n-1}^{(l_i)}(z_i) = d_i, \quad i = 0, 1, \dots, N,$$

the minimum of  $\|X_{n-1}(z)\|^2$  among all polynomials in  $\mathbb{P}_{n-1}$  satisfying the above constraints is

$$\mathbf{d}^H \mathbb{K}_{n-1}^{-1} \mathbf{d}, \quad (3.19)$$

where  $\mathbf{d}$  is the  $(N+1)$  dimensional column vector  $\mathbf{d} = (d_0, d_1, \dots, d_N)^T$ . It is clear that we need to take  $n-1 \geq N$ , otherwise the above constraints cannot be satisfied. Grenander and Rosenblatt also give the asymptotics of (3.19) when the measure

satisfies the Szegő condition and the points are inside the unit circle. Their results for constraints on the unit circle however turn out to be wrong, see [14, pp. 26].

#### 4. Recovering the discrete part outside the unit circle

Let us discuss now an application of the above results to the study of the asymptotic behavior of the discrete Sobolev orthogonal polynomials on the unit circle [2,10,11].

Let  $\mathbb{D} = \{z \in \mathbb{C}; |z| < 1\}$  be the open unit disk. The most extensively studied case of discrete Sobolev inner product corresponds to the case where  $z_k \in \mathbb{C} \setminus \overline{\mathbb{D}}$ ,  $k = 0, 1, \dots, N$ ,  $i = 0, 1, \dots, N$  (1.7). In this section, we propose a way to locate the points  $z_k$ , the masses  $M_k$ , and the order of the derivatives  $l_k$ ,  $k = 0, 1, \dots, N$ , by checking the outer relative asymptotics. In [3,6,11,10,2] and the references therein, the outer relative asymptotics of orthogonal polynomials with respect to a discrete Sobolev inner product on the unit circle was intensively studied. Here, we propose a slightly modified outline based on the results given in the previous section.

In order to obtain the asymptotic behavior of the ratio  $\psi_n(z)/\phi_n(z)$ , we need to study some asymptotic results for  $\mathbb{K}_{n-1}$  and  $\lambda_{n,n}$ .

**Lemma 4.1.** Let assume that  $d\sigma(z)$  belongs to the Nevai class and  $z_i \in \mathbb{C} \setminus \overline{\mathbb{D}}$ ,  $i = 0, 1, \dots, N$ . If  $\mathbf{b}_n = (\phi_n^{(l_0)}(z_0), \dots, \phi_n^{(l_N)}(z_N))^T$ , then

$$\lim_{n \rightarrow \infty} (\text{diag } \mathbf{b}_n)^H \mathbb{K}_{n-1}^{-1} \left( \text{diag } \mathbf{b}_n - \left( \frac{1}{z_i \bar{z}_j} \right)_{0 \leq i, j \leq N} \right) \mathbb{E}_N^{-1}.$$

**Proof.** For the kernel matrix  $\mathbb{K}_{n-1}$  given in (3.15), we have

$$\text{diag } \mathbf{b}_n \left( \text{diag } \mathbf{b}_n - \left( \frac{1}{z_i \bar{z}_j} \right)_{0 \leq i, j \leq N} \right)^H \mathbb{K}_{n-1}^{-1} \left( \text{diag } \mathbf{b}_n - \left( \frac{1}{z_i \bar{z}_j} \right)_{0 \leq i, j \leq N} \right) \mathbb{E}_N^{-1}.$$

Now, from [6] we get

$$\lim_{n \rightarrow \infty} \frac{K_{n-1}^{(l_i, l_j)}(z_i, z_j)}{\phi_n^{(l_i)}(z_i) \phi_n^{(l_j)}(z_j)} = \frac{1}{z_i \bar{z}_j - 1}, \quad (4.20)$$

and the result follows.  $\square$

**Lemma 4.2.** Let assume that  $d\sigma(z)$  belongs to the Nevai class and  $z_i \in \mathbb{C} \setminus \overline{\mathbb{D}}$ ,  $i = 0, 1, \dots, N$ . Then

$$\lim_{n \rightarrow \infty} \lambda_{n,n}^2 = \mathbf{1} + \mathbf{1} \mathbb{E}_N^{-1} \mathbf{1}^T = \lambda^{-2},$$

where  $\mathbf{1} = [1, 1, \dots, 1]$  is a  $(N+1)$  dimensional row vector.

**Proof.** From Theorem 3.1, we have

$$\lambda_{n,n}^2 = \mathbf{1} + \mathbf{b}_n^H \mathbb{I}_N + \mathbb{D}_N \mathbb{K}_{n-1} \left( \text{diag } \mathbf{b}_n - \left( \frac{1}{z_i \bar{z}_j} \right)_{0 \leq i, j \leq N} \right)^H \mathbb{D}_N \mathbf{b}_n. \quad (4.21)$$

Since [6],

$$\lim_{n \rightarrow \infty} \frac{1}{\phi_n^{(l_i)}(z_i)} = 0, \quad i = 0, 1, \dots, N,$$

when  $n$  tends to infinity we can replace in (4.21)  $(\mathbb{I}_N + \mathbb{D}_N \mathbb{K}_{n-1})^{-1}$  by  $(\mathbb{D}_N \mathbb{K}_{n-1})^{-1}$ . Thus,

$$\lim_{n \rightarrow \infty} \lambda_{n,n}^2 = \mathbf{1} + \lim_{n \rightarrow \infty} \mathbf{b}_n^H \mathbb{K}_{n-1}^{-1} \mathbf{b}_n,$$

which gives the desired result.  $\square$

We are now ready to deduce the outer relative asymptotic behavior.

**Theorem 4.1.** Let assume that  $d\sigma(z)$  belongs to the Nevai class and  $z_i \in \mathbb{C} \setminus \overline{\mathbb{D}}$ ,  $i = 0, 1, \dots, N$ . Then

$$\lim_{n \rightarrow \infty} \frac{\psi_n(z)}{\phi_n(z)} = \lambda \left[ \mathbf{1} - \mathbf{1} \mathbb{Z}_N \right],$$

where  $\mathbf{Z}_N = \left[ \frac{1}{z z_0 - 1}, \frac{1}{z z_1 - 1}, \dots, \frac{1}{z z_N - 1} \right]^T$  uniformly on every compact subset of  $\mathbb{C} \setminus \overline{\mathbb{D}} \cup \{z_0, z_1, \dots, z_N\}$ .

**Proof.** By using Theorem 3.1, we rewrite (2.10) as

$$\psi_n(z) = \lambda_{n,n} \phi_n(z) + \sum_{k=0}^n \sum_{i=0}^N \mathbf{a}_{n,i} M_i \phi_k(z) \overline{\phi_k^{(l_i)}(z_i)} \left( \lambda_{n,n} \phi_n(z) + \mathbf{a}^H \mathbb{D}_N K^{(0,l_0)}_{n-1}(z, z_0), K^{(0,l_1)}_{n-1}(z, z_1), \dots, K^{(0,l_N)}_{n-1}(z, z_N) \right)^T.$$

Therefore,

$$\frac{\psi_n(z)}{\phi_n(z)} = \lambda_{n,n} \left( \mathbf{1} - \mathbf{b}_n^H (\mathbb{I}_N + \mathbb{D}_N \mathbb{K}_{n-1})^{-1} \mathbb{D}_N (\text{diag } \mathbf{b}_n) \mathbf{K}_{n-1} \right), \quad (4.22)$$

where

$$\mathbf{K}_{n-1} = \begin{bmatrix} \frac{K^{(0,l_0)}_{n-1}(z, z_0)}{\phi_n(z) \phi_n^{(l_0)}(z_0)}, \frac{K^{(0,l_1)}_{n-1}(z, z_1)}{\phi_n(z) \phi_n^{(l_1)}(z_1)}, \dots, \frac{K^{(0,l_N)}_{n-1}(z, z_N)}{\phi_n(z) \phi_n^{(l_N)}(z_N)} \end{bmatrix}^T.$$

Notice that, when  $n$  tends to infinity, we can replace  $(\mathbb{I}_N + \mathbb{D}_N \mathbb{K}_{n-1})^{-1}$  by  $(\mathbb{D}_N \mathbb{K}_{n-1})^{-1}$  in (4.22) just as in the previous theorem. Thus, using (4.20) and Lemma 4.2 the result follows.  $\square$

If  $z = z_i$ ,  $i = 0, 1, \dots, N$  and  $\mathbf{e}_i$  denotes the column vector with entries  $\delta_{ij}$ ,  $j = 0, 1, \dots, N$ , then from the previous result we get

$$\lim_{n \rightarrow \infty} \frac{\psi_n(z_i)}{\phi_n(z_i)} = \lambda \left( \mathbf{1} - \mathbf{1} \mathbb{E}_N \mathbb{E}_N^{-1} \mathbf{e}_i \right) = \lambda \mathbf{1} - \mathbf{1} \mathbf{e}_i = 0,$$

Thus we have proved the following.

**Corollary 4.1.** Suppose that  $d\sigma(z)$  belongs to the Nevai class and  $z_i \in \mathbb{C} \setminus \overline{\mathbb{D}}$ ,  $i = 0, 1, \dots, N$ . Then

$$\lim_{n \rightarrow \infty} \frac{\psi_n(z_i)}{\phi_n(z_i)} = 0.$$

Theorem 4.1 and its corollary give a way to locate the points  $z_i$ ,  $i = 0, 1, \dots, N$ , where the derivatives in the discrete Sobolev inner product are evaluated. In order to obtain the masses  $M_i$  and the order of the derivatives  $l_i$ ,  $i = 0, 1, \dots, N$ , associated with the discrete part, we can use the following result.

**Theorem 4.2.** Suppose that  $d\sigma(z)$  belongs to the Nevai class and  $z_i \in \mathbb{C} \setminus \overline{\mathbb{D}}$ ,  $i = 0, 1, \dots, N$ . Then

$$\lim_{n \rightarrow \infty} \psi_n^{(l_i)}(z_i) \overline{\phi_n^{(l_i)}(z_i)} = \sum_{j=0}^N M_j (\mathbb{E}_N^{-1})_{ij}, \quad i = 0, 1, \dots, N.$$

**Proof.** From (2.10) and Theorem 3.1, we have

$$\begin{bmatrix} \psi_n^{(l_0)}(z_0) \\ \psi_n^{(l_1)}(z_1) \\ \vdots \\ \psi_n^{(l_N)}(z_N) \end{bmatrix} = \lambda_{n,n} \begin{bmatrix} \mathbf{b}_n + \mathbb{K}_{n-1} \mathbb{D}_N \mathbf{a}_n \\ \mathbf{b}_n + \mathbb{K}_{n-1} \mathbb{D}_N \mathbf{a}_n \\ \vdots \\ \mathbf{b}_n + \mathbb{K}_{n-1} \mathbb{D}_N \mathbf{a}_n \end{bmatrix} = \lambda_{n,n} (\mathbb{I}_N + \mathbb{K}_{n-1} \mathbb{D}_N)^{-1} \mathbf{b}_n.$$

Therefore,

$$\begin{bmatrix} \psi_n^{(l_0)}(z_0) \overline{\phi_n^{(l_0)}(z_0)} \\ \psi_n^{(l_1)}(z_1) \overline{\phi_n^{(l_1)}(z_1)} \\ \vdots \\ \psi_n^{(l_N)}(z_N) \overline{\phi_n^{(l_N)}(z_N)} \end{bmatrix} = \lambda_{n,n}^2 (\text{diag } \mathbf{b}_n)^H (\mathbb{I}_N + \mathbb{K}_{n-1} \mathbb{D}_N)^{-1} \text{diag } \mathbf{b}_n \mathbf{1}^T.$$

According to Lemma 4.1 and following the same procedure as above, we obtain



$$\lim_{n \rightarrow \infty} \begin{bmatrix} \psi_n^{(l_0)}(z_0) \overline{\phi_n^{(l_0)}(z_0)} \\ \psi_n^{(l_1)}(z_1) \overline{\phi_n^{(l_1)}(z_1)} \\ \vdots \\ \psi_n^{(l_N)}(z_N) \overline{\phi_n^{(l_N)}(z_N)} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix} \mathbf{1}^T,$$

and so our statement holds.  $\square$

From the above result, we can obtain the masses and the derivatives in the discrete part of (1.7) by checking the behavior of  $\psi_n^{(l)}(z_i) \overline{\phi_n^{(l)}(z_i)}$  for different choices of the integer  $l$ . When  $l = l_i$  the limit exists and it gives the value of the mass  $M_i$ .

## 5. Some remarks and open problems

Notice that we can derive in a straightforward way all the previous results for discrete Sobolev orthogonal polynomials on the real line, see [17]. In fact, we can say even more. Most of our results are still valid when the measure  $d\sigma(z)$  is supported on a rectifiable Jordan curve or arc in the complex plane. We restrict ourselves to the unit circle case because the statements become more transparent. From the asymptotic point of view, in [1] outer relative asymptotics have been done when the measure  $d\sigma(z)$  supported on a rectifiable Jordan curve or arc belongs to the Szegő class. In our work we have focussed our attention in a more general family of measures supported on the unit circle, the so called Nevai class that contains in a strict sense the Szegő class.

According to the above asymptotics, it is natural to ask what happens when the points  $z_i$ ,  $i = 0, 1, \dots, N$ , are located on the unit circle. The answer is well known. In any case, if  $d\sigma(z)$  belongs to the Szegő class, then using the results of [3,4] or the previous ideas, we deduce in a straightforward way that

$$\lim_{n \rightarrow \infty} \frac{\psi_n(z)}{\phi_n(z)} = 1,$$

uniformly on compact subsets of  $\mathbb{C} \setminus \overline{\mathbb{D}}$ . Obviously, our procedure to recover the discrete part of the Sobolev inner product does not hold here. Thus, a first natural question is: how to recover in this case the discrete part of our inner product?

Although the asymptotic behavior of polynomials orthogonal with respect to a discrete Sobolev has been intensively studied, there still remain some open problems to consider. What happens when the points  $z_i$ ,  $i = 0, 1, \dots, N$ , are inside the unit circle? We conjecture that, under certain conditions on  $d\sigma(z)$ , the discrete Sobolev orthogonal polynomials have the same outer asymptotic behavior as the polynomials orthogonal with respect to  $d\sigma(z)$ , when  $n$  tends to infinity.

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## References

- [1] A. Branquinho, A. Foulquié, F. Marcellán, Asymptotic behavior of Sobolev-type orthogonal polynomials on a rectifiable Jordan curve or arc, *Constr. Approx.* 18 (2002) 161–182.
- [2] A. Cachafeiro, F. Marcellán, Asymptotic behavior of Sobolev-type orthogonal polynomials on the unit circle, *J. Approx. Theory* 78 (1994) 127–146.
- [3] K. Castillo, A new approach to relative asymptotic behavior for discrete Sobolev-type orthogonal polynomials on the unit circle, *Appl. Math. Lett.* 25 (2012) 1000–1004.
- [4] K. Castillo, L.E. Garza, F. Marcellán, Asymptotic behavior of Sobolev orthogonal polynomials on the unit circle, *Integral Transforms Spec. Funct.* 24 (2013) 23–38.
- [5] T.S. Chihara, An introduction to orthogonal polynomials, *Mathematics and Its Applications*, vol. 13, Gordon and Breach, New York-London-Paris, 1978.
- [6] A. Foulquié, F. Marcellán, K. Pan, Asymptotic behavior of Sobolev-type orthogonal polynomials on the unit circle, *J. Approx. Theory* 100 (1999) 345–363.
- [7] W. Gautschi, M. Zhang, Computing orthogonal polynomials in Sobolev spaces, *Numer. Math.* 71 (1995) 159–184.
- [8] I.M. Gelfand, B.M. Levitan, On the determination of a differential equation from its spectral function, *Izv. Akad. Nauk SSSR, Ser. Mat.* 15 (1951) 309–360 (Russian); English Transl. in *Amer. Math. Soc. Transl.* (2) 1 (1955) 253–304. 26 (1975) 555–575.
- [9] U. Grenander, M. Rosenblatt, An extension of a theorem of G. Szegő and its applications to the study of stochastic processes, *Trans. Amer. Math. Soc.* 76 (1954) 112–126.
- [10] X. Li, F. Marcellán, On polynomials orthogonal with respect to Sobolev inner products, *Pacific J. Math.* 175 (1996) 127–146.
- [11] F. Marcellán, L. Moral, Sobolev-type orthogonal polynomials on the unit circle, *Appl. Math. Comput.* 128 (2002) 107–137.
- [12] F. Marcellán, A. Ronveaux, Orthogonal polynomials and Sobolev inner products. A bibliography, Universidad Carlos III de Madrid, 2012.
- [13] A. Martínez-Finkelshtein, B. Simon, Asymptotics of  $L^2$  norm of derivatives of OPUC, *J. Approx. Theory* 163 (2011) 747–773.
- [14] P. Nevai, Géza Freud, orthogonal polynomials and Christoffel functions. A case study, *J. Approx. Theory* 40 (1986) 3–167.
- [15] B. Simon, Orthogonal polynomials on the unit circle, *American Mathematical Society Colloquium Publication Series*, vol. 54, American Mathematical Society, Providence, RI, 2005 (2 vols.).

- [16] G. Szegő, Orthogonal polynomials, American Mathematical Society Colloquium Publication Series, fourth ed., vol. 23, American Mathematical Society, Providence, RI, 1975.
- [17] W. Van Assche, Sobolev-type orthogonal polynomials: how to recover the Sobolev part of the inner product, Unpublished Manuscript.
- [18] M. Zhang, Sensitivity analysis for computing orthogonal polynomials of sobolev type, in: R.V.M. Zahar (Ed.), Approximation and Computation, ISNM, vol. 119, Birkhauser Verlag, Basel, 1994, pp. 563–576.